prismatic layer is 0.35 eV/Nb atom for a d^0 count and increases slightly to 0.43 eV for a d^2 count. On the other hand, for a d^1 count we found this energy difference shrinks to 0.1 eV with the undistorted structure still favored. The shrinking of this energy difference is not unexpected in light of the known structural and electronic instabilities of analogous d^1 dichalcogenides.[28]

Acknowledgment. We thank the donors of the Petroleum Research Fund, administered by the American Chemical Society, for their partial support of this research and the National Science Foundation via NSF Grant DMR 8019741.

Appendix

All calculations were of the extended Hückel type[30] with the parameters and exponents of Table I. The weighted Wolfsberg–Helmholz formula was used.[31,32] H_{ii} values for Ru were obtained by charge iteration[33] on the actual RuO_2 net possessing a charge of $^1/_2$–/RuO_2 unit. Sources of other atomic parameters are indicated in the table. The geometrical particulars of the systems studied are described above except coordinates for $Ba_{1.14}Mo_8O_{16}$ which were graciously supplied by Professor R. McCarley. We extend thanks to Dr. Charles Torardi for providing results on $BaRu_6O_{12}$ and $K_2Mo_8O_{16}$ prior to publication.

In all calculations in crystals, matrix elements were computed between atoms separated by less than 5.94 Å. $\vec{k}$-Point meshes employed in crystalline calculations were as follows: for the two-dimensional ideal octahedral MoO_2 and NbO_2 slabs and the trigonal-prismatic NbO_2 slab, 105 $\vec{k}$ points (2-D hexagonal lattice); for the MoO_2 sheets of $Na_{0.45}Mo_2O_4$ and the analogous zigzag distorted trigonal-prismatic NbO_2 layer, 100 $\vec{k}$ points (2-D rectangular lattice); for the idealized MoO_2 and RuO_2 hollandite analogues, 40 $\vec{k}$ points (body-centered tetragonal); for the actual MoO_2 net of $Ba_{1.14}Mo_8O_{16}$, 32 $\vec{k}$ points (triclinic). Discussion of the bonding of $Na_{0.45}Mo_2O_4$ closely parallels the methodology outlined in ref 29.

Registry No. MoO_2, 18868-43-4; RuO_2, 12036-10-1; $BaMo_8O_{16}$, 52934-88-0; NbO_2, 12034-59-2.

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Contribution from the Department of Chemistry and Laboratory for Molecular Structure and Bonding,
Texas A&M University, College Station, Texas 77843

Molecular Mechanics of Low Bond Order Interactions in Tetrakis(carboxylato)dimetal Systems

JAN C. A. BOEYENS,*[†] F. ALBERT COTTON,* and SCOTT HAN

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The influence of steric factors on the lengths of metal–metal bonds of various orders has been examined by using molecular mechanics calculations. The variation in bond distances exhibited by dirhodium(II) systems, $Rh_2(XYCR)_4L_2$ (X, Y = S, O), is shown to be well explained by steric forces. Bond lengths are predicted for some as yet unknown but makable molecules. The short Rh–Rh distance in $Rh_2(O_2CCH_3)_4(H_2O)_2$ is shown to result from a compressive effect by the bridging acetate groups as proposed by Norman and Kolari. Calculations on Pd_2^{4+}, Cu_2^{4+}, and Cd_2^{4+} complexes, where it is generally accepted that no significant metal–metal bonds exist, account well for the observed metal–metal distances. Finally, a general concept for correlating bond orders, bond lengths, and bond energies in dimetal systems with a range of bond orders (0–4) is presented and discussed.

Introduction

The variation of bond length with order for bonds between metal atoms is relatively complicated compared with the behavior of simple covalent bonds.[1] This is due to the more flexible electronic configuration of transition metals and aggravated by steric interactions that occur in the fairly complicated structures often employed to stabilize metal–metal bonds of different order. Rationalization of the observed trends would be greatly facilitated by separating steric from electronic factors, and this can be achieved by the method of molecular mechanics. This model[2] treats a molecule as a set of pairwise, mechanically interacting atoms and yields an equilibrium arrangement corresponding to a minimum in the steric energy as a function of all interactions and atomic coordinates.

Our treatment begins with the (purely hypothetical) configuration that would exist if each bond length and each bond angle were individually to have the value determined only by its own intrinsic electronic properties. We then seek the *arrangement of minimum strain*, which is the one that is obtained by minimum distortion of the idealized arrangement, consistent with electronic considerations, that can be obtained without disturbance of any electronic factor. For a bond distortion this would, for instance, correspond to displacement along the characteristic potential energy Morse curve for a bond of appropriate order.[3]

The electronic factors are incorporated into the definition of the force field, which includes force constants, bond orders, and van der Waals interactions between atoms separated by a sequence of more than three chemical bonds. The force field having been adopted, all interactions are then calculated exactly. Any discrepancies between calculated and observed structure parameters must be ascribed either to an inappropriate force field or to experimental errors in the observed structure. All steric factors have now been taken into account.

Experimental Section

There is some concensus on the definition of a force field for organic molecules,[4] and although the situation is more fluid for inorganic systems, sufficient guidelines exist[5,6] to ensure that most force fields yield results that are in qualitative agreement.[7] The force field adopted for the

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Table I. Details of the Force Field

bond	*k*	r_0, Å	angle	*k*	θ_0, rad
C–H	5.0	1.08	H–C–H	0.52	1.911
C–H(arom)	5.0	1.08	H–C–C	0.65	1.911
C–C	5.0	1.54	H–C–C(arom)	0.65	2.094
C–C(arom)	7.65	1.39	C–C–C(arom)	1.0	2.094
p(C–C)arom)	0.05	2.78	C–C$\overset{\cdots}{-}$O	1.0	2.051
C$\overset{\cdots}{-}$O	5.5	1.25	C$\overset{\cdots}{-}$C$\overset{\cdots}{-}$O	1.0	2.182
C$\overset{\cdots}{-}$S	3.5	1.7	C$\overset{\cdots}{-}$O–M	0.3	2.094
C–P	3.5	1.8	C$\overset{\cdots}{-}$O–Lp	0.8	2.199
O(S)–Lp	6.0	1.0	M–O–Lp	0.4	2.094
O–Cu	0.84	1.97	C–C$\overset{\cdots}{-}$S	1.0	2.051
O–Rh	0.84	2.03	O$\overset{\cdots}{-}$C$\overset{\cdots}{-}$S	1.0	2.182
O–Pd	0.84	2.01	S$\overset{\cdots}{-}$C$\overset{\cdots}{-}$S	1.0	2.182
O–Cd	0.84	2.25	C$\overset{\cdots}{-}$S–Lp	0.8	2.199
Cu–O(ax)	0.80	2.20	C$\overset{\cdots}{-}$S–M	0.3	1.911
Rh–O(ax)	0.80	2.29	Lp–S–M	0.4	2.199
Cd–P(ax)	0.80	2.5	O–Rh–Rh	0.2	1.571
S–Rh	0.80	2.26	S–Rh–Rh	0.2	1.571
S–Pd	0.80	2.32	O–Rh–O	0.3	1.571, 3.1416
Rh–S(ax)	0.75	2.52	Cd–P–C	0.2	1.911

Table II. Torsional Potentials (kcal/mol)

torsion	*U*	torsion	*U*
M–O(S)$\overset{\cdots}{-}$C–O(S)	0.05	O(S)–Rh–Rh–O(S)	0.03
O–C–C–H	0.0146	$(\mathrm{C{-}C{-}C{-}C})_{\mathrm{arom}}$	0.1
Lp–O(S)$\overset{\cdots}{-}$C–C	0.1	$(\mathrm{H{-}C{-}C{-}H})_{\mathrm{arom}}$	0.05

Table III. Parameters of Nonbonded Interactions

interaction[a]	*a*, u	*b*, Å^{-1}	*c*, u A^6	*r*(UdW), Å
H- - -H	45.8	4.08	0.341	1.50
H- - -C	218.0	4.20	0.84	
H- - -O	239.7	4.33	0.72	
H- - -P	505.0	4.04	1.92	
H- - -S	380.0	3.94	2.18	
H- - -Cu	114.0	3.53	0.807	
H- - -M*	42.7	3.13	1.17	
C- - -C	1640.0	4.32	2.07	1.75
C- - -O	1490.0	4.45	1.77	
C- - -P	3120.0	4.16	4.73	
C- - -S	2180.0	4.05	5.38	
C- - -Cu	689.0	3.64	1.99	
C- - -M*	220.0	3.22	2.88	
O- - -O	1340.0	4.59	1.51	1.60
O- - -P	2260.0	4.28	4.04	
O- - -S	1680.0	4.18	4.60	
O- - -Cu	546.0	3.75	1.70	
O- - -M*	217.0	3.32	2.46	
P- - -P	5700.0	4.00	10.8	1.90
P- - -M*	1930.0	3.48	6.57	
S- - -S	2950.0	3.80	14.0	1.85
S- - -M*	250.0	3.02	7.48	
Cu- - -Cu	212.0	3.06	1.91	2.50
M*- - -M*	24.0	2.4	4.0	2.60

[a] M* = Rh, Pd, Cd.

present work is summarized in Tables I–III.

Table I gives force constants and strain-free values (p_0) of bond parameters. The latter depend only on inherent electronic factors prior to any influence by the steric environment. Stress on a bond is assumed to produce a harmonic deformation, with strain energy $U = {}^1/_2k(p - p_0)^2$. The force constants for bond and angle deformations are expressed in mdyn Å^{-1} and mdyn rad^{-1}, respectively.

Table II defines torsional contributions to steric strain, assumed to arise from interaction between all bonding electron groups adjacent to the reference bond. In delocalized systems this interaction is attractive and favors a torsion angle of zero. Nonplanar systems are therefore torsionally strained. All other torsional interactions are repulsive and assumed to approach zero as $\phi \to 60°$. Both types of interaction are conveniently computed by using the standard expression commonly used for calculating threefold barriers to rotation. For torsions treated individually[2] it has the form $U = {}^1/_6V(1 + 3\cos\phi)$. Appropriate values of V are listed in units of kcal mol^{-1}.

Table III provides the constants for nonbonded van der Waals interaction, described by Buckingham potentials of the type $U = ae^{-br} - cr^{-6}$. The attractive part depends on the constant *c*, which is a function of the polarizabilities and valence electron densities of the atom pair.[5] The constant *b* is a shielding function,[5] and *a* is chosen to ensure that the attractive and repulsive parts balance to produce a minimum at a separation corresponding to the sum of the van der Waals radii. Energies, *U*, are expressed in units of 10^{-11} erg/molecule ≡ kcal mol^{-1}/144. The van der Waals radii adopted for the metal atoms are our own estimates since we know of no tabulation of such radii. For more accurate work these could conceivably be refined by the analysis of accurate experimental results, but for the present application it is not justified.

Lone pairs of electrons that are sterically important have been treated as hydrogen atoms in nonbonded interactions. Their behavior in all other situations is defined in the tables.

The appropriate value of the unstrained Rh–Rh single bond was obtained by parameter adjustment, using a fixed value of 0.88 mdyn Å^{-1} for the force constant calculated by the harmonic approximation form

Table IV. Calculated and Observed Metal–Metal Distances for Different Metal and Ligand Systems

metal	M–M bond order	L_1[a]	L_2[a]	R[a]	M–M dist, Å calcd	M–M dist, Å obsd	ref
Rh	1	O	O	O	2.39	2.3855 (5)	16
		O	O	S	2.38	2.407 (1)	19
		S	O	O	2.54		
		S	O	S	2.53	2.550 (3)	17
		S	S	O	2.65		
		S	S	S	2.64		
		O	O		2.39	2.369 (6)[b]	
		S	O		2.50		
		S	S		2.59		
Pd	0	O	O		2.50	2.546 (1)[c]	13
		S	S		2.85	2.754 (1)	23
Cu	0	O	O	O	2.60	2.614 (2)	24
Cd	0	O	O	$\mathrm{PPh_3}$	3.39	3.452 (1)	15

[a] Parameters defined in Figure 1. [b] Cotton, F. A.; Wang, W., unpublished results on $\mathrm{Rh_2(O_2CCPh_3)_4}$. [c] Reported bond distance for $\mathrm{Pd_2(mhp)_4}$. See text.

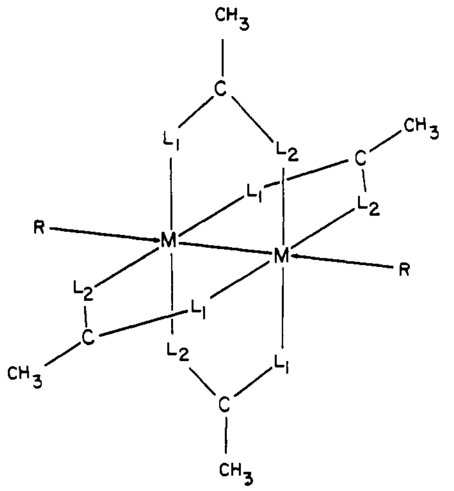

Figure 1. Schematic drawing of the bridged dinuclear systems dealt with in this work.

the observed Rh–Rh vibrational frequency[8] of 170 cm^{-1}.

A Newton–Raphson minimization coded by Boyd[9] was used for all calculations. All structures examined were based on the skeleton shown in Figure 1.

Results and Discussion

The results of the calculations are summarized in Table IV. We shall first discuss the results for the dirhodium(II) systems in which there is a formal single metal–metal bond.[10–12] The other systems (Pd, Cu, Cd) will be discussed together since they do not have a metal–metal bond.[13–15]

In the calculations for rhodium, not only the nature of the bridging donor atom (L_1, L_2) but also the axial donor atom (R) have been varied. Therefore, values obtained from the calculations include some hypothetical dirhodium(II) compounds not as yet reported in the literature. However, there is no reason why the predicted rhodium–rhodium bond lengths should not be reliable if, as it seems safe to assume, there are no additional electronic effects. Indeed, the calculated values for $Rh_2(O_2CCH_3)_4(H_2O)_2$[16] and $Rh_2(OSCCH_3)_4(CH_3CSOH)_2$[17] agree almost exactly. In fact, calculated M–M distances for all the systems agree rather well with observed values. It is therefore concluded that the variations in M–M distances in Table IV are due to purely steric factors that are governed by the nature of the bridging or axial donor atoms and groups. It is our intention to attempt the preparation of those compounds for which we have made predictions and, if this can be done, to test the predictions by determining the crystal structures.

Rhodium. The striking feature about the results for the rhodium systems is the variability of the metal–metal bond length due to steric effects. The value of r_0 for the Rh–Rh bond, that is the distance that would occur in the absence of any net steric force, was found to be 2.53 Å. The RCO_2^- ligands have the effect of drawing the metal atoms together, and somewhat surprisingly, this process is little affected (within the accuracy of the computations it is unaffected) by the presence of oxygen-type axial ligands. This bond-shortening effect of the RCO_2^- ligands is completely in accord with the proposal made by Norman and Kolari.[18]

Addition of the larger donor sulfur atom (compared with oxygen) to the dimetal unit in either bridging or axial sites causes an elongation from the value of 2.386 Å for the pure oxygen environment to 2.64 Å for the entirely sulfur-coordinated system.

We note at this juncture some important points about the groups used in the calculations. For a bridging group, the successive addition of sulfur atoms to the acetate ligand changes this first to thioacetate and then to dithioacetate. In the axial group, the change is from methanol to the methanethiol group. This is, of course, a simplification for ease in calculation, and real systems may deviate slightly from this. An example of such an effect is seen for $Rh_2(O_2CCH_3)_4(S(O)Me_2)$, where the calculated value is slightly shorter (2.384 Å) than the observed[19] distance of 2.407 Å. The slight elongation in reality is probably due to additional steric interactions of the bridging ligand system with the other groups (O, 2 CH_3) attached to the axial sulfur atom when Me_2SO is the axial ligand (as it is in reality). This deviation is small, however, and the validity of the calculations is not affected by the approximation.

The overall bond elongation of ca. 0.25 Å occurs in a stepwise fashion as a function of the donor groups. While the carboxylato groups compress the Rh–Rh bond to a minimum length because of the minimal repulsion within the ligand, the bond length increases for the thioacetate and dithioacetate compounds as the number of sterically more bulky sulfur atoms increases. Steric effects no doubt also explain the short Rh–Rh bond[20] in the methylhydroxypyridine derivative, $Rh_2(mhp)_4$, of 2.359 Å, where now the methyl groups work to compress the bond even more. It follows that because of its steric flexibility the Rh–Rh bond must be weak to allow such ligand perturbation. This is therefore a good example of where a shorter than expected metal–metal distance may not be due to strong metal–metal bonding but to a steric factor.

Pd, Cu, and Cu Compounds. A logical extension of our study of this bond-compression effect is to examine similar types of tetrakis(carboxylato) dimeric molecules in which there is no formal metal–metal bond (i.e., the M–M force constant in zero). The question of how thermodynamically stable these molecules are in view of the opposition offered by M–M repulsion against ligand compression can be addressed. In general, the calculations indicate that these dinuclear tetrakis(carboxylato) compounds are favored sterically and give wide variations in M–M bond distances due to ligand perturbations just as in the dirhodium compounds.

The case of palladium is one example of where compression by the ligand can be shown to give rise to short metal–metal distances without necessarily requiring us to invoke the formation of a bond. The hypothetical $[Pd(O_2CCH_3)_2]_n$ molecule was investigated and found to be at a minimum potential energy when the molecule is dinuclear and the Pd--Pd separation is 2.50 Å. A molecule that is similar to dinuclear palladium acetate is the $Pd_2(mhp)_4$ molecule, which has been shown[13] to have a M–M distance of 2.546 Å, in good accord with our calculated value. In reality, palladium acetate is trimeric,[21–23] but our calculations

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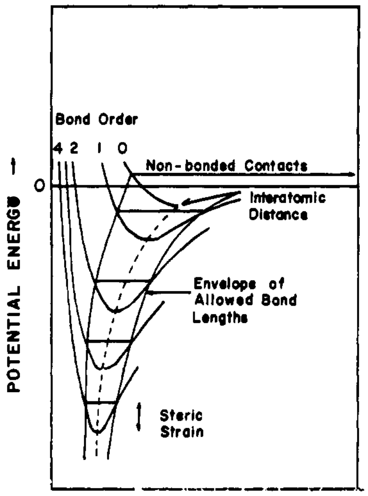

Figure 2. Qualitative representation of the relationship between bond order, bond length, and bond energy in metal–metal bonded compounds.

have shown that this trimeric form is energetically less favored. We are currently investigating additional electronic factors that may explain this seeming inconsistency.

Another palladium system of interest is the dithioacetate complex of palladium(II). The calculated distance of 2.85 Å between Pd atoms is longer than the reported[24] values of 2.754 and 2.738 Å for the two dimeric forms of $Pd_2(S_2CCH_3)_4$. The discrepancies may be due to one of two possible factors: (1) There may be an intermolecular steric repulsion from another palladium atom along the Pd--Pd axis, not taken into account in our calculation. (2) As those who reported the structure suggested,[24] there may indeed be some M–M electronic interaction along the palladium chain, also ignored in the calculation. However, the value obtained here is a good order of magnitude figure for comparison purposes.

Copper(II) tetraacetate is another example of a compound with a short metal–metal distance having a formal bond order of zero. No metal–metal bond was assumed in our calculation of bond compression by the acetate groups and axial water molecules. The figure arrived at, 2.60 Å, agrees very well with the reported[25] value of 2.614 Å in $Cu_2(O_2CCH_3)_4(H_2O)_2$.

Finally, just as the nature of the ligands can compress a dimetal center, it can also stretch the same center. One example[15] of this effect is $Cd_2(O_2CCF_3)_4(PPh_3)_2$ where the metal–metal separation reported is 3.452 Å. Our calculation, which incorporated the entire triphenylphosphine groups (with all hydrogen atoms), arrived at a M–M distance of 3.39 Å. This agreement in inter-metal distance shows the steric repulsion effect of the PPh_3 group as it works to spread out the molecule to accommodate it. Clearly, it would be of interest to know whether some other $Cd_2(O_2CR)_4L_2$ molecules with smaller L groups could be made and then to see whether they would have shorter Cd–Cd distances.

Conclusion. The observations just reported and discussed have important implications concerning the relationship between bond order and bond length. Bond order can be defined in a purely electronic way, namely as the number of bonding electrons, and therefore independent of steric factors. Bond length depends, in the first instance, on bond order, but steric factors can have a powerful modulating influence thereon, especially for low- (including zero) order bonds. Steric factors become progressively less important as the bond order increases, with concomitant increases in bond strength and force constant. This is illustrated schematically in Figure 2. It shows a family of potential energy curves representing different orders of chemical bonding between a given pair of atoms. The broken curve connecting the minima of the different bonding curves represents bond length (an inverse function of bond strength) as a function of electronic bond order only, i.e. in the absence of any steric effects. Calculations[26] of bond energy as a function of bond length are often assumed to follow relationships of this type, but they actually fail to do so because they ignore steric factors. The actual relationship cannot be described by a single curve. A given amount of steric strain deforms any of the bonds by an amount consistent with the shape of the bonding curve. The resulting envelope defines a field of possible bond lengths and bond strengths for the system, which is designated in Figure 2 as the envelope of allowed bond lengths.

Because of their lower force constant, low-order bonds are more flexible than bonds of higher order and can be either compressed or stretched by relatively large amounts, without affecting their electronic bond order. A nonbonded pair of atoms can, under some circumstances, be pushed together by a sterically cohesive molecular framework to separations similar to those expected for a comparable pair of atoms that are bonded to each other.

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Registry No. $Rh_2(O_2CCH_3)_4(H_2O)_2$, 29998-99-0; Pd_2^{4+}, 96055-81-1; Cu_2^{4+}, 96055-84-4; Cd_2^{4+}, 96055-82-2.

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